

---

Konrad-Zuse-Zentrum  
für Informationstechnik Berlin

ZIB

Takustraße 7  
D-14195 Berlin-Dahlem  
Germany

MARTIN WEISER, BODO ERDMANN, AND PETER DEUFLHARD

# **On Efficiency and Accuracy in Cardioelectric Simulation**



# On Efficiency and Accuracy in Cardioelectric Simulation

M. Weiser, B. Erdmann and P. Deuffhard

October 13, 2008

## Abstract

Reasons for the failure of adaptive methods to deliver improved efficiency when integrating monodomain models for myocardiac excitation are discussed. Two closely related techniques for reducing the computational complexity of linearly implicit integrators, deliberate sparsing and splitting, are investigated with respect to their impact on computing time and accuracy.

**AMS MSC 2000:** 65M60, 92C30

**Keywords:** cardioelectric excitation, discretization error, splitting, mass lumping

## 1 Introduction

The excitation of myocardial cells is the basis for heart contraction and thus has attracted research in modelling as well as simulation. The propagation of a depolarization front of the transmembrane potential through the myocardium ultimately leads to the release of  $\text{Ca}^{2+}$  and thus a contraction of the muscle fibers. The evolution of the transmembrane potential is described by a set of reaction-diffusion equations modeling the ion transport by anisotropic diffusion between cells as well as between intra- and extracellular space (cf. [10, 11, 12]).

Under the simplifying assumption of identical intra- and extracellular diffusion tensor, myocardial excitation is described by the monodomain equation linking the transmembrane potential  $v$  to gating variables  $w$  and ion concentrations  $c$ :

$$c_m \partial_t v = \text{div}(D_M \nabla v) + I_{\text{ion}}(v, w, c) \quad (1)$$

$$\partial_t w = R(v, w) \quad (2)$$

$$\partial_t c = S(v, w, c) \quad (3)$$

The reactions  $I_{\text{ion}}$ ,  $R$ , and  $S$  are specified by membrane models. Here we restrict our attention to a very small phenomenological model by Aliev and Panfilov [1] and a physiological model by Luo and Rudy [7] of moderate complexity.

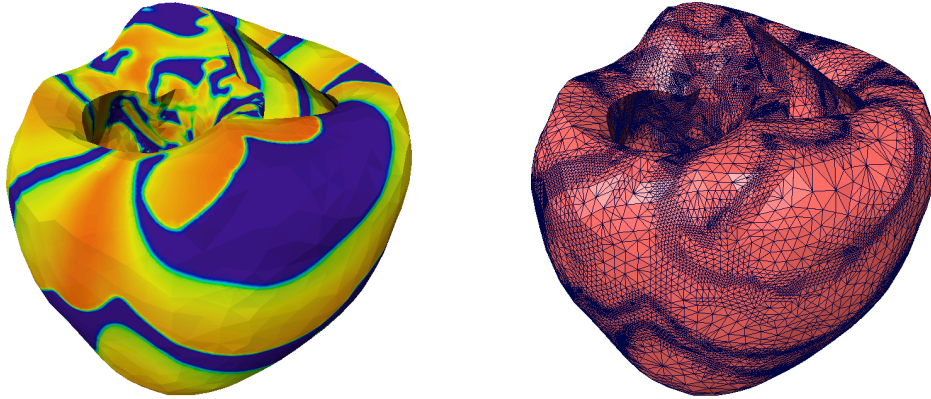


Figure 1: Typical front of potential in ventricular fibrillation and the corresponding adaptive mesh.

## 2 Adaptive Integration of Reaction-Diffusion Equations

The most common approach to spatial discretization of (1)–(3) is to use finite element methods on a fixed, quasi-uniform mesh. Due to the small width of the depolarization front relative to the heart geometry, rather fine meshes are needed in order to obtain sufficiently accurate solutions. Recently, adaptive FE methods have been proposed for simulating the myocardial excitation [3, 13, 2, 5].

The results reported e.g. in [5] using the fully adaptive, linearly implicit FE code KARDOS [6] are mixed. On one hand, error control works just as expected and the number of vertices encountered in adaptive mesh refinement is a factor 150 below the number of vertices in a uniform mesh achieving the same local resolution (see Fig. 1 for illustration). On the other hand, the reduction in the number of degrees of freedom is not translated into savings of computing time, which is unacceptably high.

There seem to be several reasons for this effect. First of all, as long as a depolarization front is traversing the domain, the time step is limited by front speed and width. Only when the whole domain is covered by the plateau phase, the time step increases significantly. In the fibrillation example computed in [5], at any point in time there is a depolarization front somewhere in the domain, such that the time step remains small. Second, error control and mesh adaptation require the computation of an error estimator, which takes a significant part of the computational work. Third, mesh modifications require the frequent assembly of stiffness and mass matrices, up to a few times each time step. Finally, mesh modifications themselves and the resulting non-locality of data structures take their toll.

### 3 Deliberate Sparsing

Rosenbrock methods, which are linearly implicit Runge-Kutta methods, are used in KARDOS for time stepping. The lowest order method is the linearly implicit Euler scheme

$$(I - \tau(J + \nabla \cdot D\nabla))u_{k+1} = u_k + \tau(f(u_k) - Ju_k) \quad \text{with } J = f'(u_k) \quad (4)$$

for solving  $\partial_t u = \text{div}(D\nabla u) + f(u)$ .

When applied to the monodomain equations (1)–(3), the linear system (4) has to be solved with a nonsymmetric block matrix

$$J_{AP} = \begin{bmatrix} M - \tau(\partial_v f_v + A) & -\tau \partial_w f_v \\ -\tau \partial_v f_w & M - \tau \partial_w f_w \end{bmatrix} \quad \text{or} \quad J_{LR} = \begin{bmatrix} * & * & * & * & * & * & * & * \\ * & * & & & & & & \\ * & & * & & & & & \\ * & & & * & & & & \\ * & & & & * & & & \\ * & & & & & * & & \\ * & & & & & & * & \\ * & & & & & & * & * & * \end{bmatrix}$$

for the Aliev-Panfilov and Luo-Rudy membrane models, respectively.  $A$  denotes the stiffness matrix whereas  $M$  stands for the mass matrix.  $*$  denotes a non-zero matrix with the sparsity structure of  $M$ . One problem with Rosenbrock methods is that their convergence order is reduced if the linear systems corresponding to (4) is not solved exactly.

A subset of linearly implicit methods, so-called W-methods (cf. [4]), allows to use arbitrary matrices  $J \neq f'$  without affecting the order of convergence. This enables *deliberate sparsing* [9], a technique to drop certain parts of  $f'$  in order to decrease the computational complexity in computing  $J$  and solving the system. Even though in principle the error constant is affected by the approximation error  $J - f'$ , in practice the step sizes depend mostly on how well the large negative eigenvalues are captured. This is because stability limits the step size for explicit methods. Numerical experiments indicate that for normal heart beat cycle and both models, the system's stiffness is dominated by the diagonal blocks, such that dropping all off-diagonal blocks is possible without decreasing step size. The remaining block diagonal  $B$  is not only smaller, but also symmetric, which allows to use more efficient methods for symmetric matrices. Nevertheless, time savings given in Tab. 1 are disappointing. The reason for this is not yet clear and under investigation.

### 4 Splitting and Mass Lumping

Another sparsing opportunity on the element level comes from the fact that no spatial derivatives are involved in the reactions  $R$  and  $S$ . Instead of using the FE

framework for propagating the gating variables and ion concentrations, their values can be computed spatially decoupled by solving the ODE at each mesh vertex. This is known as *splitting* [8], leaving just a  $1 \times 1$  FE "block" system to be solved.

From a different point of view, *mass lumping* by using quadrature rules with nodes only at the element vertices when assembling the mass matrices is an established method to obtain diagonal mass matrices. Of course, diagonal mass matrices are easily stored and trivially inverted. A closer inspection reveals that splitting leads to diagonal blocks in the notation of Section 3 as well. Moreover, splitting and mass lumping are mathematically equivalent, which permits a seamless interpretation of splitting in the framework of FE. Due to the lower accuracy of the vertex-based quadrature, the a-priori error estimates are worse for mass lumping than for Gaussian quadrature with nodes in the interior of the elements. While the FE convergence order is the same, the discretization error may be increased by a constant factor. In different contexts, factors of 4–6 are usually observed. Since an  $L^2$ -error reduction of 4 requires one additional level of uniform refinement, splitting may be expected to require an 8 times larger discretization than using a full FE approach with more accurate quadrature.

A closer look at the spatial discretization errors of the gating variables and ion concentration reveals a more subtle influence of splitting on the total accuracy. Variables with slow dynamics are spatially smooth, whereas fast variables follow the depolarization front quickly and exhibit strong local features. On the same spatial grid, the discretization error in the slow variables is therefore very small, and an error increase by a factor of four has little effect on the overall solution. In contrast, for fast variables the effect is clearly visible (see Fig. 2). Comparable results are obtained with adaptive computations on 3D domains. Unfortunately,

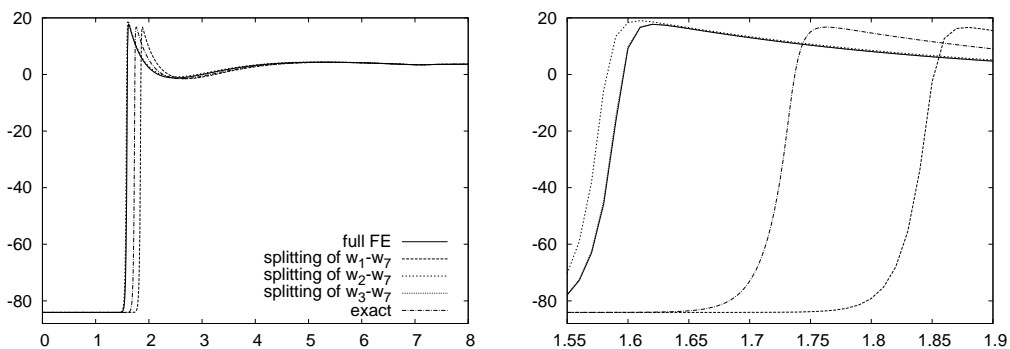


Figure 2: Depolarization front positions 0.1s after ignition at the right hand side boundary of the 1D domain for splitting of different groups of gating variables in the Luo-Rudy model. Left: whole domain. Right: zoom. The full FE solution travels faster than the exact solution. Mass lumping for the fastest gating variable  $w_1$  has the largest effect and slows down the front even behind the exact solution.

alg. feature	Aliev-Panfilov	Luo-Rudy
deliberate block sparsing	1.05	1.25
splitting $w_1-w_7$	2	30
splitting $w_2-w_7$		15
splitting $w_3-w_7$		4

Table 1: Wall-clock runtime reduction factors due to algorithmic improvements in KARDOS.

when mass lumping is only done for a subset of the gating variables, the runtime improvements are less pronounced (see Tab. 1).

Surprisingly, the integration of gating variables without any spatial discretization error is actually possible — at least on fixed grids. The key observation is that with a given quadrature rule for assembling the reaction terms in (1), the gating variables are only evaluated at a finite set of points in the domain  $\Omega$ . Propagating the gating variables just at these spatial positions yields exact values, up to time discretization, as far as the transmembrane potential is affected. Even more surprisingly, the overall accuracy of the front speed obtained with quasi-exact gating values can be worse than a full FE approach using the same quadrature rule, see Fig. 3 left. Increasing the accuracy of the quadrature rule gives results which are quite similar to the full FE approach, see Fig. 3 right, which indicates that the dominating discretization error is due to the transmembrane potential.

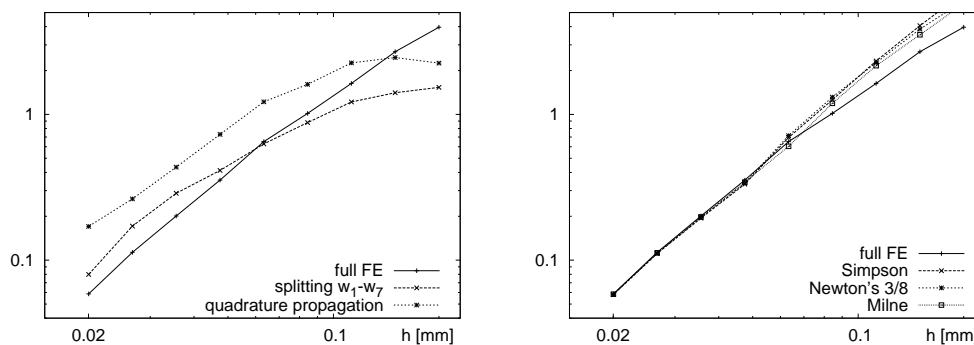


Figure 3: Depolarization front position error on a 1D domain after 0.1s of simulating the Luo-Rudy model with different mesh sizes. Left: full FE, mass lumping, and propagating at Gauß quadrature nodes. The errors, closely related to the front speed errors, span a range of about factor 3. Right: Effect of different quadrature rules.

## 5 Conclusions

Adaptive discretization of cardioelectric excitation yields reliable results with a relatively small number of degrees of freedom, but the overhead of error estimation, mesh adaptation and frequent assembly on modified grids outweighs the efficiency gains. Deliberate sparsening and splitting techniques can improve the situation to some extent, but their effect on accuracy needs to be investigated in more detail.

## References

- [1] R.R. Aliev and A.V. Panfilov. A simple two-variable model of cardiac excitation. *Chaos, Solitons and Fractals*, 7:293–301, 1996.
- [2] Y. Belhamadia. A time dependent adaptive remeshing for electrical waves of the heart. *IEEE Transact. Biomed. Eng.*, 55(2):443–452, 2008.
- [3] P. Colli Franzone, P. Deuffhard, B. Erdmann, J. Lang, and L.F. Pavarino. Adaptivity in space and time for reaction-diffusion systems in electrocardiology. *SIAM J. Sci. Comput.*, 28(3):942–962, 2006.
- [4] P. Deuffhard and F.A. Bornemann. *Scientific Computing with Ordinary Differential Equations*. Texts in Applied Mathematics, vol. 42. Springer, 2<sup>nd</sup> edition, 2002.
- [5] P. Deuffhard, B. Erdmann, R. Roitzsch, and G.T. Lines. Adaptive finite element simulation of ventricular dynamics. *Comput. Vis. Sci.*, to appear.
- [6] J. Lang. *Adaptive Multilevel Solution of Nonlinear Parabolic PDE Systems*, volume 16 of *Lecture Notes in Computational Science and Engineering*. Springer, 2001.
- [7] C. Luo and Y. Rudy. A model of the ventricular cardiac action potential: depolarization, repolarization, and their interaction. *Circ. Res.*, 68(6):1501–1526, 1991.
- [8] M. Munteanu and L.F. Pavarino. Decoupled Schwarz algorithms for implicit discretizations of nonlinear monodomain and bidomain systems. *Math. Mod. Meth. Appl. Sci. (M3AS)*, to appear.
- [9] U. Nowak. Dynamic sparsening in stiff extrapolation methods. *IMPACT Comput. Sci. Engrg.*, 5:53–74, 1993.
- [10] A.V. Panfilov and A.V. Holden, editors. *Computational Biology of the Heart*. Wiley, 1997.



- [11] F.B. Sachse. *Computational Cardiology*, volume 2966 of *Lecture Notes in Computer Science*. Springer, 2004.
- [12] J. Sundnes, G.T. Lines, X. Cai, B.F. Nielsen, K.-A. Mardal, and A. Tveito. *Computing the Electrical Activity in the Heart*, volume 1 of *Monographs in Computational Science and Engineering*. Springer, 2006.
- [13] J.P. Whiteley. Physiology driven adaptivity for the numerical solution of the bidomain equations. *Annals of Biomed. Engrg.*, 35(9):1510–1520, 2007.